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SXPS Studies of Ta_2O_5-Al_2O_3 Alloys For Si-FET Gate Dielectric Applications

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Beamline(s): U4A

Introduction: High dielectric constant (high-k) materials are being considered as alternatives for thermal SiO_2 in Si-FET applications to enable sub-1nm gate oxides with increased reliability and reduced leakage. The interfacial electronic structure of these high-k gate oxide films is important for a fundamental understanding of the properties of these material systems. Ta_2O_5-Al_2O_3 alloys have an electronic structure typical of high-k gate dielectrics. The synchrotron X-ray photoelectron spectroscopy (SXPS) available at beamline U4A is ideal for interface studies of sub-1nm films.

Methods and Materials: The SXPS configuration at U4A includes a six meter spherical grating monochromator which yields a photon beam with an energy resolution of less than 0.1eV over the range of 10 to 300eV. Photoelectron kinetic energy is measured with a VSW 100mm hemispherical analyzer fixed at 45^o to the photon beam axis. Thin films of Al_2O_3, Ta_2O_5 and their alloys were deposited by remote plasma enhanced chemical vapor deposition (RPECVD) and annealed at North Carolina State University. The Si 2p, Al 2p, Ta 4f and valence spectra of Al_2O_3, Ta_2O_5 and alloys with 34%, 43% and 76% Ta_2O_5 were acquired. Spectra were fit with models based on physical assumptions regarding the films.

Results: Figure 1 shows the complimentary auger electron spectroscopy (done at North Carolina State University) and SXPS analysis of Al 2p core state energies. The Al 2p energies shift toward higher energy as the alloy composition changes from Al_2O_3 to Ta_2O_5. The Ta 4f states shift in a similar fashion. The small shift in the SXPS data is consistent with the small difference in electronegativity of the end member oxides. Figure 2 shows the comparison of Si 2p 3/2 SXPS spectra for Al_2O_3 and SiO_2 thin films. All alloy compositions have a similar Si 2p spectrum. The similarity between the two spectra in fig. 2 indicates that i) an intermediary SiO_2 layer is formed between the Al_2O_3 and the Si substrate, and ii) suboxide bonding is qualitatively similar to SiO_2-Si bonding. The Si^{4+} peak is shifted to lower binding energy and is broader than the Si^{4+} peak for a SiO_2 layer without a high-k dielectric overlayer. This is attributed to i) a modification of the Si^{4+} photohole screening due to the high-k dielectric overlayer and ii) the presence of a silicate bonding (Si-O-Al) at the Al_2O_3/SiO_2 interface.

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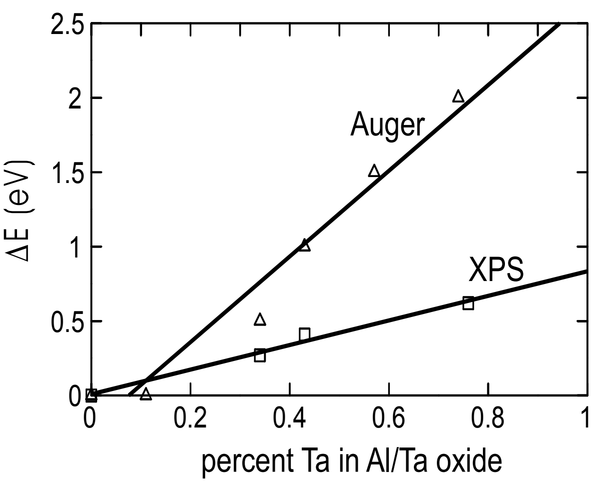

Figure 1. Al 2p 3/2 shift due to increased Ta_2O_5.

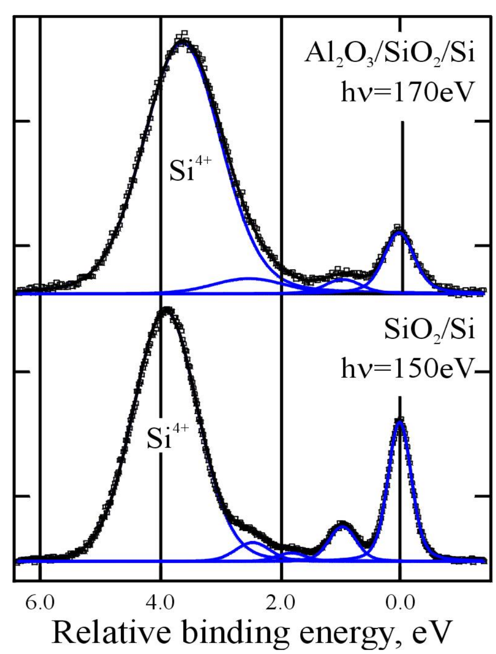

Figure 2. Si 2p 3/2 SXPS spectra for Al_2O_3 and comparison with SiO_2.